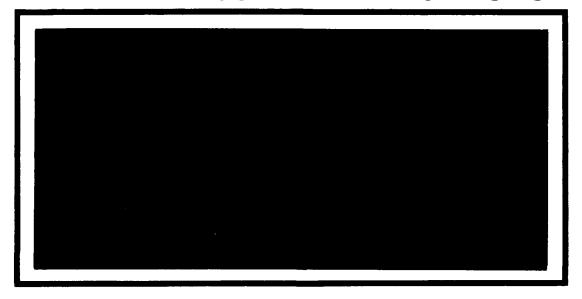




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On the Theory and Error Estimation of the Reduced Basis Method for Multi-Parameter Problems<sup>1</sup>

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### On the Theory and Error Estimation of the Reduced Basis Method for Multi-Parameter Problems<sup>1</sup>

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#### WERNER C. RHEINBOLDT<sup>2</sup>

ABSTRACT. In an earlier paper (ZAMM 63, 1983, 21), J.P.Fink and W.C.Rheinboldt developed a priori local error estimates for the scalar-parameter case of the reduced basis method by considering the method in a differential-geometric setting. Here it is shown that an analogous setting can be used for the analysis of the method applied to problems with a multi-dimensional parameter vector and that this leads to a corresponding local error theory also in this general case.

#### 1. Introduction.

The computational analysis of many problems in science and engineering involves the solution of very large systems of nonlinear equations. Thus, not surprisingly, there is considerable interest in reducing the size of these problems. One of these reduction techniques has become generally known as the reduced basis method. Some early work on this method includes [N77], [ASB78], but, beginning with [NP80], [N81], [N82], [NP83a], much of the detailed development for a range of problems in nonlinear structural mechanics is due to A. Noor and his co-workers. Since then the literature on the method has grown rapidly and also the number of application-areas has grown and includes now, for instance, initial value problems for ordinary differential equations ([PL87]), differential-algebraic equations ([L91]), certain classes of parabolic differential equations ([J90]), as well as climate problems ([JM87], [M88]).

The method applies to systems of parametrized, nonlinear equations and was originally developed in the setting of a standard continuation procedure for nonlinear problems with

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one scalar parameter. But, in [NP83b], [NBS84], [NPA84], [NAT87], A. Noor et al showed that it can also be extended to problems involving several parameters. A first, general analysis of the a priori error behavior of the method in the one-parameter case was given in [FR83]. Some further aspects of these results were discussed in [P85], and then in [FR85] a general local error estimation theory was developed which contains the earlier estimates as special cases. The approach in [FR83] was to place the method in a general differential geometric setting where it can be formulated as a projection onto a subspace spanned by the first several vectors of the moving frame of the solution path.

In this paper we show that this geometric approach can be extended to the multiparameter case. For this we summarize in section 2 the indicated differential geometric setting and then show in section 3 that the general local error theory of [FR85] can be applied to the multi-parameter case of the reduced basis method. This is followed in section 4 with a discussion of the basic approach to the computation of the reduced basis vectors which turns out to correspond to that developed by A. Noor (loc.cit.) by different means. At the same time, the theory suggests some new computational approaches for low-order approximations.

#### 2. The Basic Setting.

As noted above, many stationary problems in technical applications are modelled by a nonlinear equation

$$(2.1) F(z,\lambda) = 0$$

involving a state variable z; a d-dimensional parameter vector  $\lambda$ ; and a differential operator F with associated boundary conditions. Standard discretizations – for instance, by finite elements or finite differences – typically produce very large finite-dimensional nonlinear systems of equations. The aim of the reduced basis method is to construct special approximations that reduce the number of degrees of freedom without compromising the errors.

 The equation (2.1) involves a mapping  $F: Z \times \Lambda \to Y$  from the product  $Z \times \Lambda$  of the state space Z and parameter space  $\Lambda$  into another space Y. Typically, the solution set

$$(2.2) M = \{ (z, \lambda) \in Z \times \Lambda; \ F(z, \lambda) = 0 \}$$

is a differentiable submanifold of  $Z \times \Lambda$ . All standard discretizations leave the parameters unchanged and hence produce approximate equations of the form

$$(2.3) F_h(z_h, \lambda) = 0$$

involving a mapping  $F_h: Z_h \times \Lambda \to Y_h$  where  $Z_h \subset Z$  and  $Y_h \subset Y$  are suitably chosen finite dimensional subspaces. The construction of  $Z_h$ ,  $Y_h$ , and  $F_h$  usually takes little or no account of the properties of the solution manifold M. Hence, in our differential-geometric terminology, the idea of the reduced basis method may be viewed as the design of approximations that do take account of information about the manifold M and its local coordinate systems.

For a classical illustration of this idea, suppose that  $M \subset \mathbb{R}^3$  constitutes a smooth curve

$$x:J\subset R^1\to R^3,\quad x=x(s)\in R^3,\ s\in J.$$

It is no restriction to assume that s denotes here the arclength. Then the local moving frame at x = x(s) consists of the tangent vector  $u_1(s) = x'(s)$ , the principal normal  $u_2(s) = x''(s)/||x''(s)||_2$ , and the bi-normal vector  $u_3(s) = u_1(s) \times u_2(s)$ . If we express x locally near  $x(s_0)$  in terms of this moving frame,

$$x(s) = x(s_0) + \sum_{k=1}^{3} \alpha_k(s, s_0) u_k(s_0),$$

then the coefficients satisfy the well known approximation properties

$$\alpha_k(s, s_0) = (x(s) - x(s_0))^T u_k(s_0) = O((s - s_0)^k), \quad k = 1, 2, 3, \text{ as } s \to s_0.$$

Analogously, a sufficiently smooth curve in  $R^n$  can be approximated locally to order k+1 by using as coordinate system the first k moving frame vectors,  $1 \le k \le n$ . In other words, independent of the dimension n of the ambient space, already a few basis vectors may suffice to represent the curve locally to a relatively high accuracy. This is the fundamental idea behind the reduced basis approximations.

As noted above, the given equation (2.1) generally models a problem in an infinite dimensional state space Z. Then, in essence, we have the following two possible choices for introducing the desired approximation:

- (a) Use a 'reduced-basis' approximation of the solution manifold (2.2) of the original, infinite-dimensional equation (2.1).
- (b) Construct first a standard discretized equation (2.3) of the original problem and then choose a 'reduced-basis' approximation of the solution manifold of this discretized equation.

Evidently, (a) has the advantage of only one small discrete problem and hence only one discretization error. But, in general, this approximation is difficult to obtain since it requires working directly with the original infinite dimensional equation. In contrast, (b) has the advantage that the 'reduced-basis' approximation is much easier to compute since it involves only finite dimensional equations. But there is now the disadvantage that the first discrete system (2.3) is large and that the resulting two discretization errors are hard to control together. Despite of this, (b) has become the generally accepted approach.

3. The Local Error Estimation. In line with the approach (b) we assume from now on that

$$X,Y$$
 real, linear spaces with dim  $X=n,$  dim  $Y=m,$   $n=m+d,$   $d\geq 1;$  (3.1)

 $F: S \to Y$ ,  $C^{\rho}$ -mapping on the open set  $S \subset X$ ,  $\rho \geq 2$ .

In other words, F represents the first discretization of the original operator. Generally, for any linear space E we denote an open or closed neighborhood of a point  $e \in E$  by  $\mathcal{U}(e, E)$  or  $\bar{\mathcal{U}}(e, E)$ , respectively. On all linear subspaces of E the relative topology is used.

As usual, a point  $x^0$  is a regular point of the mapping F if rank  $DF(x^0) = m$ . Suppose that as the result of some computations we have accepted a regular point  $x^0 \in S$  and that  $F(x^0) = y^0$ . Then the submersion theorem ensures that for a sufficiently small neighborhood  $\mathcal{U}(x^0, X) \subset S$  the local solution set

(3.2) 
$$M = \{ x \in \mathcal{U}(x^0, X); F(x) = y^0 \}$$

is a  $C^{\rho}$ -submanifold of X of dimension d.

In order to introduce a local parametrization of this manifold at  $x^0$  we choose a splitting

(3.3) 
$$X = T \oplus V$$
, dim  $T = d$ , dim  $V = m$ ,  $V \cap \ker DF(x^0) = \{0\}$ .

and consider the equation  $F(x^0+t+v)=y^0$  with  $t\in T$  and  $v\in V$ . Evidently, (3.3) implies that  $DF(x^0)_{|V}\in \text{Isom }(V,Y)$ . Hence the implicit function theorem ensures the existence of neighborhoods  $\mathcal{U}(0,V)$  and  $U_{\Phi}=\mathcal{U}(0,T)$  with  $\mathcal{U}(x^0,X)=x^0+U_{\Phi}+\mathcal{U}(0,V)\subset S$  and of a  $C^{\rho}$ -map  $v:U_{\Phi}\to V$  with v(0)=0 such that the local coordinate map

(3.4) 
$$\Phi: U_{\Phi} \to X, \quad \Phi(s) = x^0 + t + v(t), \ t \in U_{\Phi},$$

is a  $C^{\rho}$ -diffeomorphism from  $U_{\Phi}$  onto the (relatively) open neighborhood  $\mathcal{U}(x^0, X) \cap M$  of  $x^0$  in M (see also [R86]).

A projection method will be used to construct the desired approximation of the manifold M. For this let

(3.5a) 
$$P_p \in L(V), P_p^2 = P_p, \text{ rge } P_p = V_p, \text{ dim } V_p = p < m,$$

be a given projection and note that, because of dim  $V = \dim Y = m$  we can choose a linear mapping

$$(3.5b) \hspace{1cm} J \in L(X,Y), \hspace{3mm} \ker J = T, \hspace{3mm} \operatorname{rge} J = Y, \hspace{3mm} J_{|V} \in \operatorname{Isom}(V,Y).$$

Then the subspace  $X_p = T \oplus V_p \subset X$  has dimension d+p, and  $\Pi_p = J_{|V}P_pJ_{|V}^{-1} \in L(Y)$  is a projection of Y onto the subspace  $Y_p = \text{rge } \Pi_p = J_{|V}V_p$  of dimension p. Thus the approximate problem

(3.6a) 
$$F_p: S_p = S \cap (x^0 + X_p) \to Y_p, \quad F_p(x) = \Pi_p F(x), \ x \in S_p,$$

(3.6b) 
$$F_p(x) = y_p^0, \quad x \in S_p, \ y_p^0 = \Pi_p y^0.$$

is well defined.

Obviously,  $x^0 \in S_p$  not only satisfies the original equation  $F(x) = y^0$  but also the approximate equation (3.6b). We are interested in the solutions of (3.6b) locally near  $x^0$  and in an estimate of the approximation error. For this we extend the mapping (3.6a) to all of S in line with the following result:

Lemma 1. Consider the extended mapping

(3.7) 
$$\hat{F}_p: S \to Y, \quad \hat{F}_p(x) = (I_Y - \Pi_p) J_{|V} \Gamma(x - x^0) + \Pi_p(F(x) - y^0),$$

where  $\Gamma \in L(X)$  denotes the natural projection of  $X = T \oplus V$  onto the second factor. Then  $\hat{F}_p(x) = 0$  for some  $x \in S$  if and only if  $x \in S_p$  and  $F_p(x) = y_p^0$ .

The proof is straightforward. In fact, if  $\hat{F}_p(x) = 0$  for  $x = x^0 + t + v \in S$  then  $J_{|V}v = \prod_p (J_{|V}v - F(x) + y^0) \in Y_p$  whence  $v \in V_p$  and therefore  $x \in S_p$  as well as  $(I_Y - \prod_p)J_{|V}v = 0$  and  $F_p(x) = y_p^0$ . Conversely, if  $F_p(x) = y_p^0$  for  $x = x^0 + t + v \in S_p$  then  $v \in V_p$  and thus  $\hat{F}_p(x) = 0$ .

Evidently, we have  $\hat{F}_p(x^0) = 0$  and it turns out that  $x^0$  is a regular point of  $\hat{F}_p$  if the condition

(3.8) 
$$V_p \cap \ker \Pi_p DF(x^0) = \{0\},$$

holds. In fact, by (3.7) we have

$$D\hat{F}_{p}(x^{0}) = (I_{y} - \Pi_{p})J_{|V}\Gamma + \Pi_{p}DF(x^{0})$$

and (3.8) shows that  $DF_p(x^0)_{|V_p} \in \text{Isom } (V_p, Y_p)$  whence  $\Pi_p DF(x^0)$  maps V onto  $Y_p$  while  $(I_y - \Pi_p)J_{|V|}\Gamma$  maps V onto the complement rge  $(I_y - \Pi_p)$ . Therefore, all points x in some sufficiently small neighborhood  $\mathcal{U}(x^0, X) \subset S$  of  $x^0$  are regular and the local solution set

(3.9) 
$$M_{p} = \{ x \in \mathcal{U}(x^{0}, X); \hat{F}_{p}(x) = 0 \},$$

is again a d-dimensional submanifold of X of class  $C^{\rho}$ .

It turns out that, because of (3.8), we can define the approximation error by comparing points on M and  $M_p$  near  $x^0$  that have the same coordinate t. This leads to the following theorem proved in [FR85] (see also [R86]):

Theorem 1. Under the assumptions (3.1) let  $x^0 \in S$ , with  $F(x^0) = y^0$ , be a regular point where on the local manifold M of (3.2) the splitting (3.3) defines the local coordinate map (3.4). With the projection (3.5a) and the linear map (3.5b) introduce the approximate problem (3.7a/b) and suppose that (3.8) holds. Then there exists a ball  $B_0 \subset U_{\Phi}$  centered at the origin of T and a neighborhood U(0, V) such that  $x^0 + B_0 + U(0, V) \subset S$  and that for any  $t \in B_0$  the equation  $\hat{F}_p(x^0 + t + w) = 0$  has a unique solution  $w = v_p(t)$  in U(0, V). The mapping  $v_p : B_0 \to U(0, V)$  is of class  $C^p$  and satisfies  $v_p(B_0) \in V_p \cap U(0, V)$ . Moreover, the error estimate

(3.11) 
$$||v(t) - v_p(t)|| \le C||(I_V - P_p)v(t)||, \quad \forall t \in B_0,$$

holds with a constant C independent of t.

We sketch briefly the proof and refer for further details to [FR85] or [R86]. It is based on the following implicit function theorem used, in a more general form, in [BRR81a,b,c]:

Theorem 2. Let V, T, Y be finite dimensional, real, linear spaces and  $G: S \to Y$  a  $C^{\rho}$ map,  $\rho \geq 2$ , on an open set S of  $X = T \times V$  with  $(0,0) \in S$  and G(0,0) = 0. Suppose that
on a compact neighborhood  $U_c = \bar{U}(0,T)$  there exists a Lipschitz - continuous function  $v: U_c \to V$  such that v(0) = 0,  $t + v(t) \in S$  for  $t \in U_c$ , and

- (i)  $D_vG(t,v(t)) \in Isom(V,Y), \forall t \in U_c$ ,
- (ii)  $||D_v G(t, v(t))^{-1}|| \le \gamma_1$ ,  $||D_t G(t, v(t))|| \le \gamma_2$ ,  $\forall t \in U_c$ ,
- (iii)  $\lim_{t\to 0} ||G(t,v(t))|| = 0$ ,

where  $\gamma_1$ ,  $\gamma_2$  are positive constants independent of t. Then there exists a ball  $B_0 \subset U_c$  centered at the origin of T and a neighborhood  $\mathcal{U}(0,V)$  such that  $B_0 \otimes \mathcal{U}(0,V) \subset S$  and that for any  $t \in B_0$  the equation G(t,w) = 0 has a unique solution  $w = w(t) \in \mathcal{U}(0,V)$ . Moreover, the mapping  $w: B_0 \to V$  is of class  $C^\rho$  and

$$||w(t) - v(0)|| \le C||t||, \quad \forall t \in B_0$$

with a constant C independent of t.

The main part of the proof of Theorem 1 consists in applying Theorem 2 to the mapping

$$G: S_G = \{(t, v); t \in T \times V, x^0 + t + v \in S\} \to Y, \quad G(t, v) = \hat{F}_p(x^0 + t + v).$$

By Lemma 1 we have G(t,v)=0 for  $(t,v)\in S_G$  exactly if  $x=x^0+t+v\in S_p$  and  $F_p(x)=y_p^0$ . Moreover, (3.8) implies that  $D_vG(0,0)\in \mathrm{Isom}\,(V,Y)$ . Hence

$$D_v G(t,v) \in \text{Isom } (V,Y), \|D_v G(t,v)^{-1}\| \le \alpha_1, \|D_t G(t,v)\| \le \alpha_2,$$

for all (t, v) in some compact neighborhood  $\tilde{U}((0, 0), T \times V) \subset S_G$ . We restrict this neighborhood such that for all  $(t, v_1), (t, v_2) \in \tilde{U}((0, 0), T \times V)$ 

$$||G(t,v_2)-G(t,v_1)-D_vG(t,v_1)(v_2-v_1)|| \leq \frac{1}{2\alpha_1}||v_2-v_1||.$$

whence it follows readily that

$$(3.13) ||v_2-v_1|| \leq \frac{\alpha_1}{2} ||G(t,v_2)-G(t,v_1)||, \quad \forall (t,v_1), (t,v_2) \in \bar{U}((0,0), T \times V),$$

Since the mapping  $v:U_{\Phi}\to V$  in (3.4) is of class  $C^{\rho}$  and v(0)=0 there exists a compact neighborhood  $U_c=\bar{U}(0,T)\subset U_{\Phi}$  such that  $(t,v(t))\in\bar{U}((0,0),T\times V)$  for  $t\in U_c$ . This implies that the conditions (i) and (ii) of Theorem 2 hold on  $U_c$ . Moreover, (iii) is a direct consequence of

$$\|\hat{F}_p(\Phi(t))\| = \|(I_Y - \Pi_p)J_{|V}\Gamma(\Phi(t) - x^0)\| \le \text{const } \|(\Phi(t) - x^0)\|.$$

Thus Theorem 2 applies and there exists a ball  $B_0 \subset U_{\Phi}$  centered at the origin of T and a neighborhood  $\mathcal{U}(0,V)$  such that  $x^0 + B_0 + \mathcal{U}(0,V) \subset S$  and that for any  $t \in B_0$  the equation  $\hat{F}_p(x^0 + t + w) = 0$  has a unique solution  $w = v_p(t)$  in  $\mathcal{U}(0,V)$ . Moreover, the mapping  $v_p: B_0 \to \mathcal{U}(0,V)$  is of class  $C^p$  and it follows from Lemma 1 that  $v_p(B_0) \in V_p \cap \mathcal{U}(0,V)$ . Finally, (3.12) ensures that  $||v_p(t)|| \leq C||t||$  for  $t \in B_0$ . Hence, by restricting, if needed, the ball  $B_0$  we have  $(t,v(t)), (t,v_2) \in \bar{\mathcal{U}}((0,0), T \times V)$  and the estimate (3.11) follows directly from (3.13).

#### 4. The Choice of the Reduced Basis Vectors.

The local error estimate (3.11) suggests that we should construct the approximating space  $V_p$  such that the quantity

(4.1) 
$$||(I_V - \Pi_p)v(t)||$$

is as small as possible. For this we consider at the given regular point  $x^0 \in S$  the 'tangential' splitting

$$(4.2) X = T \oplus V, T = \ker DF(x^0), V = \operatorname{rge} DF(x^0)^T.$$

for which (3.2) certainly holds. Here we may use

$$(4.3) J = DF(x^0) \in L(X,Y).$$

as the mapping (3.5b). The term 'tangential' splitting derives from the fact that the tangent space of the local solution manifold (3.2) of F at  $x^0$  may be identified with  $\ker DF(x^0)$ .

For the computation we need basis mapping s

$$(4.4) K \in L(R^d, X), rge K = T,$$

and

$$(4.5) A \in L(\mathbb{R}^p, X), \quad \text{rank } A = p, \quad \text{rge } A = V_p \subset V.$$

of the local parameter space T and the approximating space  $V_p$ , respectively. By the choice (4.3) of J we have  $JA \in L(\mathbb{R}^p, Y)$  and rank JA = p whence there exists a bi-orthogonal mapping

$$(4.6) B \in L(R^p, Y), \quad B^T J A = I_p,$$

and, the corresponding projections  $P_p$  and  $\Pi_p$  can be written as

$$(4.7) P_p = AB^T J, \quad \Pi_p = JAB^T.$$

Therefore the resulting approximate equation is equivalent with the reduced problem

(4.8) 
$$G(s,w) \equiv B^T F(x^0 + Ks + Aw) = b^0 \equiv B^T y_p^0, \quad G: R^d \times R^p \to R^p.$$

The condition (3.8) is here automatically satisfied. In fact, if  $\Pi_p DF(x^0)u = 0$  for some  $u \in V_p$  then, since JAw = 0 only if w = 0, we have  $B^TDF(x^0)u = 0$  and therefore  $u \in \ker DF(x^0) \cap V_p \subset \ker DF(x^0) \cap V = \{0\}$ .

For the representation of the local coordinate map (3.4) it is useful to introduce the mapping

(4.9) 
$$\eta: \mathcal{U}(0, \mathbb{R}^d) \to Y, \quad \eta(s) = DF(x^0)^+ v(Ks), \ s \in \mathcal{U}(0, \mathbb{R}^d),$$

where as usual  $DF(x^0)^+ = (DF(x^0)DF(x^0)^T)^{-1}DF(x^0)$  and hence  $DF(x^0)DF(x^0)^+$  is the orthogonal projection onto V. Then we have  $v(Ks) = DF(x^0)^T\eta(s)$  for  $s \in \mathcal{U}(0, \mathbb{R}^d)$ . The tangency property of the splitting obviously implies that  $D\eta(0) = 0$ . Thus for any k less than the differentiablity class  $\rho$  of F we obtain

(4.10) 
$$v(Ks) = \sum_{j=2}^{k} \frac{1}{j!} DF(x^0)^T D^j \eta(0) s^{(j)} + \mathcal{R}(s), \quad s \in U_0 = \mathcal{U}(0, \mathbb{R}^d)$$

where the remainder  $\mathcal{R}(s)$  satisfies

(4.11) 
$$\|\mathcal{R}(s)\| = O(\|s\|^{k+1}), \quad \text{as } \|s\| \to 0$$

and we used the notation  $s^{(j)} = (s, s, \dots, s), (j$ -times).

Therefore, if we choose the approximating space  $V_p$  such that for some  $k \geq 2$ 

$$(4.12) DF(x^0)^T D^j \eta(0) s^{(j)} \in V_p, \quad j = 2, \dots, k, \ \forall s \in \mathbb{R}^d.$$

then it follows from (4.10) and (4.11) that

(4.13) 
$$||(I_V - \Pi_p)v(Ks)|| = ||\mathcal{R}(s)|| = O(||s||^{k+1}), \quad \text{as } ||s|| \to 0,$$

and we obtain from Theorem 1 the desired asymptotic estimate

$$(4.14) ||v(Ks) - v_p(Ks)|| = O(||s||^{k+1}), \text{ as } ||s|| \to 0.$$

For fixed  $s \in U_0$  the mapping

(4.15) 
$$\tau \in \mathbb{R}^d, \ |\tau| < \delta \quad \mapsto \quad \gamma_s(\tau) = x^0 + \tau K s + D F(x^0)^T \eta(\tau s)$$

defines a path on M through  $x^0$  which has at  $x^0$  the derivatives

(4.16) 
$$D\gamma_s(0) = t = Ks, \quad D^j\gamma_s(0) = DF(x^0)D^j\eta(0), \ j = 2,\ldots,\rho.$$

The natural inner-product of X induces on  $M_0$  a Riemannian structure and the derivatives (4.16) reflect geometric properties of this Riemannian manifold near  $x^0$ . For example, the second orde, term satisfies

$$DF(x^{0})^{T}D^{2}\eta(0)s^{(2)} =$$

$$(4.17) \qquad = -DF(x^{0})^{T}[DF(x^{0})DF(x^{0})^{T}]^{-1}D^{2}F(x^{0})t^{(2)} = \mathcal{V}(t,t), \ t = Ks \in T$$

where  $\mathcal{V}$  denotes the second fundamental tensor of  $M_0$  at  $x^0$  (see [RR89]) and hence this term reflects curvature properties of  $M_0$ . Similarly

$$DF(x^0)^T D^3 \eta(0) s^{(3)} = D^3 F(x^0) t^{(3)} + 3D^2 F(x^0) (t, \mathcal{V}(t, t) - DF(x^0) t,$$

represents a first "torsion" tensor.

Since  $F(\gamma_s(\tau)) = 0$  for sufficiently small  $\tau \in \mathbb{R}^d$ , it follows by repeated differentiation that

(4.18) 
$$DF(x^0)D^j\gamma_s(0)s^{(j)} = H_j(x^0)t^{(j)}, \quad t = Ks \in T, \ j = 2, \dots, k,$$

with multi-linear operators  $H_j(x^0)$  that are readily calculated recursively. For example, we have

$$\begin{split} &H_2(x^0)t^{(2)} = -D^2F(x^0)t^{(2)}, \\ &H_3(x^0)t^{(3)} = -D^3F(x^0)t^{(3)} + 3D^2F(x^0)(t, D^2\gamma_s(0)s^{(2)}). \end{split}$$

For the computation of the derivatives  $D^j\gamma(0)s^{(j)}$  occurring in  $H_3, H_4, \ldots$  note that because of  $K^T\gamma_s(t) = K^T(x^0 + \tau Ks)$  for  $\tau \in R^d$  we have  $K^TD^j\gamma_s(0) = 0$  for  $j = 2, \ldots, k$ . Therefore, these derivatives are the unique solutions of the systems

(4.19) 
$$\left( \frac{DF(x^0)}{K^T} \right) D^j \gamma_s(0) s^{(j)} = \left( \frac{H_j(x^0) t^{(j)}}{0} \right), \quad t = Ks \in T, \ j = 2, \dots, k$$

since, by construction of K, the matrix

$$\binom{DF(x^0)}{K^T}$$

is nonsingular. The systems (4.19) were derived differently by A.Noor et al (see e.g. [NR83]) who also showed them to be an effective tool for the computation of the needed path derivatives for many practical problems. For a related discussion about some of the numerical aspects we refer also to [M87].

For the construction of the approximating subspace  $V_p \subset X$  that satisfies the condition (4.12), let  $s_1, s_2, \ldots, s_d$  be some basis of  $R^d$  and compute for given k the

$$\hat{p} = \begin{pmatrix} d+k \\ k \end{pmatrix} - d - 1$$

vectors

$$(4.21) DF(x^0)^T D^j \eta(0)(s_1^{(i_1)}, \dots, s_j^{(i_j)}) \in X, \quad i_1 + \dots + i_j = j, \ j = 2, \dots, k.$$

These vectors span the desired subspace  $V_p \subset X$ . In practice, we usually finds that its dimension p equals  $\hat{p}$  in which case the vectors (4.21) can be used directly as the columns of the matrix A. Otherwise, there are various means of extracting a linearly independent subset to construct A.

Besides the  $\hat{p}$  vectors (4.21) we need d vectors for K. In view of (4.20) the total number  $d + \hat{p}$  of vectors that have to be computed, increases very rapidly as the following table shows:

k	d = 1	d=2	d=4	d=6	d = 10
1	1	2	4	6	10
2	2	5	14	27	65
3	3	9	34	83	285
4	4	14	69	209	1000

For practical applications this limits the reduced basis approach to problems with a small number d of parameters and to a choice of small orders of approximation k. But the

use of small k, say k = 2 or k = 3, obviously requires more frequent updates of the basis vectors which in turn calls for the development of faster algorithms for the computation of these vectors.

We conclude this discussion by showing that for k = 2 the relation (4.6) with the second fundamental tensor of M leads to a direct algorithm for computing K, A, and B based on the results of [RR90]. For this suppose that natural bases are used on  $X = R^d$  and  $Y = R^m$ . With the QR-factorization

$$DF(x^0)^T = (Q_1, Q_2) \begin{pmatrix} R \\ 0 \end{pmatrix}$$

where rge  $Q_2 = \ker DF(x^0)^T$ , we can set  $K = Q_2$ . For any given  $s \in \mathbb{R}^d$  with sufficiently small  $||t|| \le \epsilon$  let  $x = x^0 + Ks$ . Then the chord Newton algorithm

while "no convergence"

solve 
$$R^T z = F(x)$$
 for  $z$ ;

$$set x := x - Q(z,0)^T;$$

converges to  $\Phi(s) = x^0 + Ks + DF(x^0)^T \eta(s) \in M$  and hence implements the tangential coordinate system.

The algorithm of [RR90] for computing the second fundamental tensor assumes that the natural inner product is used to induce a Riemannian structure on the manifold M. Briefly, for d=2 and k=2 let  $u_1$  and  $u_2$  denote the two columns of  $K=Q_2$  and set  $u_3=u_1+u_2$ . It was shown in [RR90] that for  $u=u_i$  with fixed index i=1,2,3, and any sufficiently small h>0 the algorithm

$$y_1 = \Phi(h)$$
 chord Newton process  $y_2 := \Phi(-h)$  chord Newton process  $v := (y_1 - x^0) + (y_2 - x^0)$  approximation of the normal vector  $v := v - u_i^T v u_i$  orthogonalization w. r. t.  $u_i$   $v := v/\|v\|$  normalization to length 1

produces an approximation of  $v_i = V(u_i, u_i)$ . With  $W = (v_1, v_2, v_3)$  we compute now the

singular value decomposition of the  $3 \times 3$  matrix JW:

$$\begin{pmatrix} B_0^T \\ B_1^T \end{pmatrix} JW(C_0, C_1) = \begin{pmatrix} \operatorname{diag} (\sigma_1, \dots, \sigma_p) & 0 \\ 0 & 0 \end{pmatrix}.$$

Here we have  $B_0 \in R^{m \times p}$  and  $C_0 \in R^{3 \times p}$  and  $p \leq 3$  denotes the maximal index such that  $\sigma_1 \geq \ldots \geq \sigma_p > 0$ . Then it follows that  $p = \operatorname{rank} A$  and hence that

$$A = WC_0$$
,  $B = B_0 \operatorname{diag}(1/\sigma_1, \dots, 1/\sigma_n)$ .

are the desired basis matrices.

The algorithm can be efficiently integrated into the method for computing simplicial approximations of M developed in [R88]. This also opens up the possibility of extending the approach to the case d=2, k=3 by using finite difference approximations for computing the required third order basis vectors. The resulting overall process will be explored elsewhere.

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